2,2-Bis(bromomethyl)-1,3-propanediol

3296-90-0 | DTXSID9020164

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.72e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.59e-01

Confidence level: 3.54e-01

Nearest Neighbors from the Training Set

Image not found
Oxydemeton-methyl
Measured: 15.0
Predicted: 2.58e-05

Image not found
Diethylene glycol
Measured: 3.23e-03
Predicted: 5.76e-03

Image not found
Dicofol
Measured: 1.00e-04
Predicted: 2.79e-07

Image not found
3-Methylaniline
Measured: 4.89e-04
Predicted: 2.01e-01

Image not found
3-Pentanone
Measured: 2.00e-01
Predicted: 29.7